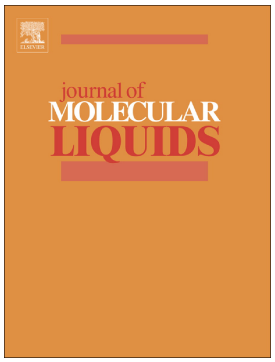

A molecular dynamics study on the melamine aqueous solution

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A Molecular Dynamics Study on the Melamine Aqueous Solution

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Abstract

The molecular dynamics simulations and density functional theory have been performed to investigate the melamine (MEL) aqueous solution at different concentrations and temperatures. We have studied the microscopic structure of MEL aqueous solution, dielectric properties, hydrogen-bond dynamics and the transportation properties. The MEL molecules weakly distorted the tetrahedral structures and the hydration shells have not been observed, which means that water molecules in the MEL aqueous solution find themselves is not a very unusual environment from that in the pure water. The temperatures dependent on the water structure, the permittivity, hydrogen-bond numbers and hydrogen-bond lifetimes decrease with the temperatures increase, and vice versa for the diffusion coefficient. At high-frequency, the vibrational power specturm is consistent with the experiment.

Keywords: Tetrahedral structure; Hydration shells; Hydrogen-bond dynamics; MEL aqueous solution

1. Introduction

MEL, 1,3,5-triazine-2,4,6-triamine is a trimer of cyanamide and its structural schematic illustration is shown in the Fig. 1[1, 2]. It has been widely applied in industrial chemistry, laminates, glues, adhesives, flame retardants and plastics [3, 4] because of the nitrogen-rich nature[5, 6]. However, since the illegal added scandal had been reported at 2008 in China [4, 7-11], it has been found that the MEL has no nutritive value and cannot take the place of protein [12], and the excessive MEL will

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